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QUANTUM MOTION ON TWO PLANES CONNECTED AT ONE POINT

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1. Introduction

The theory of self-adjoint extensions found recently some new applications[1-5]. It can be particularly useful in the situations when the configuration manifold of a quantum system consists of a few parts which are "glued" together in some way. An example of this type has been treated in our previuos paper[6]; we consider there a particle moving freely on a halfline connected to a plane. Such a study has a straightforward physical motivation, because it yields a mathematical model for one type of point contacts, the spear-and-anvil contact[7].

There is another characteristic experiment in the quantum point-contact spectroscopy, in which two metallic plates are separated by a thin insulating layer perforated at one point. If the size of the orifice is comparable with the mean free path of the electrons in metal, the Ohm's law is violated and one observes non-linear effects in the current-voltage characteristics[7]. One can conceive various mathematical models of this situation. The simplest among them treats electrons as free particles moving on the manifold consisting of two planes connected in one point. That is the problem we are going to discuss in the present letter.

We shall construct, by means of self-adjoint extensions, the family of all possible Hamiltonians for such a system, and characterize them by singular boundary conditions. Then we shall find to each particular Hamiltonian the probability of penetration between the two planes. It yields the basis for evaluation of the current-voltage characteristics[8] which will be performed in a subsequent paper.

2. The family of admissible Hamiltonians

For simplicity, we neglect spin of the electrons. The state Hilbert space of our problem is then $\mathcal{H} = L^2(\mathbb{R}^2) \oplus L^2(\mathbb{R}^2)$. In order to construct the Hamiltonians, we start with the operator

$$H_0 = H_{0,1} \oplus H_{0,2} \quad , \tag{1}$$

where $H_{0,j} = -\Delta$ with $D(H_{0,j}) = C_0^\infty(\mathbb{R}^2 \setminus \{0\})$, $j = 1,2$, assuming the connection point to be placed at the centre of coordinates at each of the planes. The used notation is more or less standard - cf., e.g., Ref.9 . The deficiency indices of the operators $H_{0,j}$ are known [6] to be (1,1) ; hence the deficiency indices of H_0 are (2,2) and it possesses a four-parameter family of self-adjoint extensions. The deficiency subspaces $\mathcal{K}^\pm = \mathrm{Ker}(H_0^* \mp iI)$ are spanned by the vectors $\varphi_k^{(\pm)}$, $k = 1,2$, where

$$\varphi_1^{(+)} = (f_0, 0) \quad , \quad \varphi_2^{(+)} = (0, f_0) \tag{2a}$$

with

$$f_0(x) = H_0^{(1)}(\varepsilon|x|) \quad , \quad \varepsilon = e^{\pi i/4} \tag{2b}$$

and $\varphi_k^{(-)}$ are complex conjugated to $\varphi_k^{(+)}$. In order to construct the extensions, it is useful to introduce polar coordinates in each of the planes and decompose $L^2(\mathbb{R}^2) = \bigoplus_{m=-\infty}^{\infty} L^2(\mathbb{R}^+, r\,dr) \otimes \{Y_m\}_{\mathrm{lin}}$, where $Y_m(\varphi) = (2\pi)^{-1/2} e^{im\varphi}$. The operators $H_{0,j}$ can be then expressed as

$$H_{0,j} = \bigoplus_{m=-\infty}^{\infty} h_{m,j} \otimes I \quad , \tag{3a}$$

where

$$h_{m,j} = -\frac{d^2}{dr^2} - \frac{1}{r}\frac{d}{dr} + \frac{m^2}{r^2} \quad , \quad D(h_{m,j}) = C_0^\infty(\mathbb{R}^+ \setminus \{0\}) \quad . \tag{3b}$$

Since the operators $h_{m,j}$ are e.s.a. for $m \neq 0$ (Ref.9, Sec.X.1), we have

Proposition 1 : Each self-adjoint extension of H_0 is of the form

$$H_U = K_U \oplus \bar{h} \quad , \tag{4}$$

where $h = (\bigoplus_{m\neq 0} h_{m,1} \otimes I) \oplus (\bigoplus_{l \neq 0} I \otimes h_{l,2})$ and K_U is a self-adjoint extension of the operator $K_0 = (h_{0,1} \otimes I) \oplus (I \otimes h_{0,2})$ with the domain $D(K_0) = \{ \varphi = (f_1, f_2) \; : \; f_j(x) = \tilde{f}_j(|x|) \; , \; \tilde{f}_j \in C_0^\infty(\mathbb{R}^+ \setminus \{0\}) \}$.

Hence it's only necessary to find K_U. The standard von Neumann theory gives

Proposition 2 : The extensions K_U are parametrized by 2×2 unitary matrices U . We have

$$K_U(f_1,f_2) = \left(-\frac{d^2 f_1}{dr^2} - \frac{1}{r}\frac{df_1}{dr} \, , \, -\frac{d^2 f_2}{dr^2} - \frac{1}{r}\frac{df_2}{dr}\right) \tag{5a}$$

and

$$D(K_U) = \{ f = \psi + c_1(\varphi_1^{(+)} + u_{11}\varphi_1^{(-)} + u_{12}\varphi_2^{(-)}) + c_2(\varphi_2^{(+)} + u_{21}\varphi_1^{(-)} + u_{22}\varphi_2^{(-)}) \; : \; \psi \in D(\bar{K}_0) \; , \; c_1, c_2 \in \mathbb{C} \} . \tag{5b}$$

3. Boundary conditions

It is useful to characterize the extensions H_U by means of boundary conditions. The deficiency functions are singular, but we can introduce the regularized boundary values [6,10]

$$L_0(f) = \lim_{r\to 0} \frac{f(r)}{\ln r} \quad , \quad L_1(f) = \lim_{r \to 0} \left[f(r) - L_0(f) \ln r \right] \; . \tag{6a}$$

In particular, the standard expansion of Hankel functions yields

$$L_0(f_0) = \frac{2i}{\pi} \quad , \quad L_1(f_0) = \frac{1}{2} + \frac{2i}{\pi}(\gamma - \ln 2) \tag{6b}$$

and complex conjugated values for $L_j(\bar{f}_0)$, where $\gamma = 0.577216...$ is the Euler's constant. One must also split the set of all matrices U into five disjoint classes, namely

(i) all U with $D(U) \equiv \mathrm{tr}\,U - \det U - 1 \neq 0$,

(ii) all non-diagonal U with $D(U) = 0$,

(iii) and (iv) : the matrices $\begin{pmatrix} 1 & 0 \\ 0 & e^{i\omega} \end{pmatrix}$ and $\begin{pmatrix} e^{i\omega} & 0 \\ 0 & 1 \end{pmatrix}$ with $\omega \in (0, 2\pi)$,

(v) the unit matrix.

Proposition 3 : Every extension K_U is specified uniquely by the following boundary conditions. If $f = (f_1, f_2)$ belongs to $D(K_U)$, then

(i) $L_1(f_1) = AL_0(f_1) + BL_0(f_2)$ and $L_1(f_2) = CL_0(f_1) + DL_0(f_2)$, where

$$A = \frac{\pi i}{4}(1 + u_{11} - u_{22} - \det U)D(U)^{-1} + \gamma - \ln 2 \quad ,$$

$$B = \frac{\pi i}{2} u_{21} D(U)^{-1} \quad , \quad C = \frac{\pi i}{2} u_{12} D(U)^{-1} \quad ,$$

$$D = \frac{\pi i}{4}(1 - u_{11} + u_{22} - \det U)D(U)^{-1} + \gamma - \ln 2 \quad ,$$

(ii) $L_0(f_2) = EL_0(f_1)$ and $L_1(f_2) = FL_0(f_1) + GL_1(f_1)$, where

$$E = u_{12}(u_{11}-1)^{-1} = u_{21}^{-1}(u_{22}-1) \quad ,$$

$$F = \frac{\pi i}{2}\, u_{21}^{-1}\left[\frac{1}{2}\,\mathrm{tr}\,U + \frac{2i}{\pi}(\gamma - \ln 2)(1-\det U)\right] \quad ,$$

$$G = u_{12}(1-u_{22})^{-1} = u_{21}^{-1}(1-u_{11}) \quad ,$$

(iii-v) if $U = \begin{pmatrix} e^{i\omega_1} & 0 \\ 0 & e^{i\omega_2} \end{pmatrix}$, the boundary conditions read $L_1(f_j) = (\frac{\pi}{4}\,\mathrm{ctg}\,\frac{\omega_j}{2} + \gamma - \ln 2)L_0(f_j)$, in particular, $L_0(f_j) = 0$ if $\omega_j = 0$.

<u>Proof</u> : The boundary conditions are obtained by straightforward computation from (2),(5b) and (6b). Next one has to check that the mapping from the set of the matrices U to the set of boundary conditions is injective ; it can be done in the same way as in the proof of theorem of Sec.3 in Ref.6. ∎

4. <u>Scattering at the connection point</u>

It is clear from Proposition 3 that the boundary conditions separate for a diagonal U . The Hamiltonian is therefore of the form $H_U = H_{0,1}^{(A)} \oplus H_{0,2}^{(D)}$, where the operators on the rhs are two-dimensional point-interaction Hamiltonians/11/. The electron cannot penetrate between the two planes ; the scattering problem in each of them can be considered separately.

We are more interested in the case when the penetration is possible. Suppose that U <u>is non-diagonal</u> and <u>belongs to the class (i)</u>. We take the function f^U with

$$f_1^U(r) = J_0(kr) + a_U(k)H_0^{(1)}(kr) \quad , \quad f_2^U(r) = b_U(k)H_0^{(1)}(kr) \qquad (7)$$

and require it to belong locally to $D(H_U)$; a short calculation then gives

$$a_U(k) = \frac{1 + \frac{2i}{\pi}(\gamma + \ln\frac{k}{2} - D)}{\left[1+\frac{2i}{\pi}(\gamma+\ln\frac{k}{2}-A)\right]\left[1+\frac{2i}{\pi}(\gamma+\ln\frac{k}{2}-D)\right] + \frac{4}{\pi^2}\,BC} \quad , \qquad (8a)$$

$$b_U(k) = \frac{2i}{\pi}\, C \left[1+\frac{2i}{\pi}(\gamma+\ln\frac{k}{2}-D)\right]^{-1} a_U(k) \quad . \qquad (8b)$$

Using the asymptotics of the functions (7) for $r \to \infty$, one finds

$$S_0(k) \equiv e^{2i\delta_0(k)} = 1 + 2a_U(k) =$$
$$= \frac{\left[-1+\frac{2i}{\pi}(\gamma+\ln\frac{k}{2}-A)\right]\left[1+\frac{2i}{\pi}(\gamma+\ln\frac{k}{2}-D)\right] + \frac{4}{\pi^2}\,BC}{\left[1+\frac{2i}{\pi}(\gamma+\ln\frac{k}{2}-A)\right]\left[1+\frac{2i}{\pi}(\gamma+\ln\frac{k}{2}-D)\right] + \frac{4}{\pi^2}\,BC} \quad , \qquad (9)$$

while the other $\delta_m(k)$ are easily seen to be zero ; only the s-wave scattering is non-trivial. Using an explicit parametrization/6/ of the matrix U , one can check that the coefficients A,D are real and $\bar{B} = C$. Then a straightforward calculation shows that S is non-unitary,

$$1 - |S_0(k)|^2 = 4\,|b_U(k)|^2 > 0 \quad . \qquad (10a)$$

This relation has a natural interpretation. In order to illustrate it, one has to calculate the radial probability current through the circle of radius r in the second plane. It equals

$$j(r) = -2\pi r\,|b_U(k)|^2\ \mathrm{Im}\left[H_0^{(2)}(kr)\,k\,H_1^{(1)}(kr)\right] = 4\,|b_U(k)|^2 \qquad (10b)$$

independently of r ; hence the rhs of (10a) is the probability of penetration through the connection point per unit time. This is just the quantity needed for the model mentioned in the introduction.

Analogous considerations can be performed for U <u>of the class (ii)</u>. In particular, the relations (8) are now replaced by

$$a_U(k) = \frac{G}{(E-G)\left[1+\frac{2i}{\pi}(\gamma+\ln\frac{k}{2})\right] - \frac{2i}{\pi}\,F}$$

and $b_U(k) = Ea_U(k)$, and the s-wave scattering matrix is

$$S_0(k) = \frac{E+G+\frac{2i}{\pi}(E-G)(\gamma+\ln\frac{k}{2}) - \frac{2i}{\pi}\,F}{E-G+\frac{2i}{\pi}(E-G)(\gamma+\ln\frac{k}{2}) - \frac{2i}{\pi}\,F} \quad .$$

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Квантовое движение на двух плоскостях, соединенных в одной точке

Рассматривается свободное движение частицы на многообразии, состоящем из двух плоскостей, соединенных в одной точке. Четырехпараметрическое семейство допустимых гамильтонианов строится при помощи самосопряженных расширений свободного гамильтониана, из которого удалена особая точка. Вычислена вероятность прохождения частицы между двумя частями конфигурационного многообразия. Результаты применимы для одной модели квантовой контактной спектроскопии.

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Quantum Motion on Two Planes Connected at One Point

We study free motion of a particle on the manifold which consists of two planes connected at one point. The four-parameter family of admissible Hamiltonians is constructed by self-adjoint extensions of the free Hamiltonian with the singular point removed. The probability of penetration between the two parts of the configuration manifold is calculated. The results can be used as a model for quantum point-contact spectroscopy.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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